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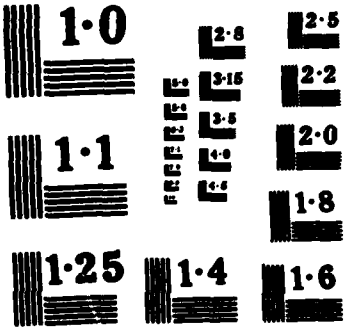

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THEORETICAL CALCULATIONS SUPPORTING INVESTIGATION OF METAL CONTACTS TO ULTRASMALL SEMICONDUCTOR STRUCTURES

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Interim Report

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The aim of this Interim Report is to describe the research progress made during the first part of the Project DAJA 45-84-M-0378.

The main objective of this project is to perform ab initio electronic structure calculations of the metal-III-V semiconductor interface as the semiconductor layer becomes very thin (a superlattice). These calculations might result in guiding the experimental efforts made by other groups to develop and understand metal contacts to these layers. Let us stress, however, that the proposed collaboration with the experimental groups has not yet been implemented due to different problems in the experimental efforts of the aforementioned groups.

The analysis of the electronic structure of metal-III-V semiconductor superlattice contacts is the objective of this work. In particular, we are interested in the barrier height of the contact and its electronic density of interface states. Compared with the usual metal-semiconductor junctions [1], we have the additional problem associated with the different interfaces of the superlattice, which can interfere with the metal contact. We shall consider the following structure:

metal - m layers of SC_1 - n layers of SC_2 -
- m layers of SC_1 - n layers of SC_2 - ...,

along the (100) semiconductor direction. In particular, we propose to analyse the following superlattices: GaAs-AlAs [2] and InAs-GaSb [3], forming the following contacts with Ga:

$$\ldots - \underbrace{Ga - Ga}_{\text{Metal}} - \underbrace{Ga - As}_{SC_1} - \underbrace{Al - As}_{SC_2} - \underbrace{Ga \ldots}_{SC_1}$$

$$\ldots\text{-}\underbrace{Ga-Ga}_{\text{Metal}}-\underbrace{Ga-Sb}_{SC_1}-\underbrace{In-As}_{SC_2}-\underbrace{Ga-Sb}_{SC_1}-\ldots$$

$$\ldots\text{-}\underbrace{Ga-Ga-Ga}_{\text{Metal}}-\underbrace{Sb-Ga}_{SC_1}-\underbrace{As-In}_{SC_2}-\underbrace{Sb-Ga}_{SC_1}-\ldots,$$

where we take m = n = 4 or 5, corresponding to very thin superlattice layers.

The metal and the semiconductor electronic structures will be analysed by means of a tight-binding model, which has been shown to be appropriate for analysing the usual metal-semiconductor junctions [4]. In this procedure, it is essential to introduce the interface self-consistency associated with the rearrangement of the interface charge; this can be achieved by means of appropriate perturbations introduced in the interface layers. A similar method has to be applied to the metal-superlattice junction. In this case, self-consistency has to be introduced in the metal-semiconductor and the semiconductor$_1$-semiconductor$_2$ interfaces. Accordingly, we propose to analyse the metal-superlattice junction in the following steps:

(i) First of all, we shall analyse the semiconductor$_1$-semiconductor$_2$ junction by introducing the appropriate perturbations at the interface. It is an easy matter to show that, for this case, we can apply the same method developed for the metal-semiconductor junction. The main point is to calculate self-consistently the interface perturbation, the rearrangement of charge and the interface dipole [5].

(ii) In a second step, we shall consider the self-consistency associated with the metal-semiconductor interface. In this case we shall follow literally the procedure developed in Ref.4.

(iii) Finally, we shall analyse the full metal-superlattice junction by assuming that the different pieces of self-consistency as calculated in steps (i) and (ii) are not modified by the interference of the different interfaces. This has been shown to be a good approximation [6]. However, the electronic levels and the barrier height of the junction are strongly dependent on the interference among the different interfaces. We shall calculate this effect on the electronic structure of the junction in a final step.

At this moment we are completing the calculation of step (i) for the two superlattices given at the beginning of this report, and we are planning to start with step (ii) in one month time.

Delivery Schedule

Although this first Interim Report was required before 30 November 1984, we have had difficulties to comply with this date due to problems in developing the contact with the experimental groups. Accordingly, we ask for the following extension of the delivery schedule:

Second Interim Report: *15 June 1985*, instead of 30 March 1985,
Final Report: *30 October 1985*, instead of 30 August 1985.

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